The energy states of quantum dots through the variational method and SQM*

Elso Drigo Filho
Instituto de Biociências, Letras e Ciências Exatas, IBILCE-UNESP
Rua Cristovão Colombo, 2265 - 15054-000 São José do Rio Preto - SP

Regina Maria Ricotta
Faculdade de Tecnologia de São Paulo, FATEC/SP-CEETPS-UNESP
Praça Fernando Prestes, 30 - 01124-060 São Paulo-SP
Brazil

Abstract

The Variational Method is applied within the context of Supersymmetric Quantum Mechanics to provide information about the energy states of a hydrogenic donor in a quantum dot.

I. INTRODUCTION

Twenty years ago Supersymmetric Quantum Mechanics (SQM) appeared inside the study of the SUSY breaking mechanism of higher dimensional quantum field theories, [1]. Since then it has been considered as a new field of research, providing not only a supersymmetric interpretation of the Schrödinger equation, but interesting answers to all sorts of non-relativistic quantum mechanical systems. Particular points to be mentioned include the better understanding it brought of the exactly solvable, [2]- [3], the partially solvable, [4], [**?**], the isospectral, [6], [7], the periodic, [8] and the non-exactly solvable potentials, [9]- [11]. The latter were studied by the association of the variational method with SQM formalism. The scheme employed in them is based on an *ansatz* made to the superpotential. Through the superalgebra it is possible to evaluate the wave function, the trial wave function, which contains the free parameters that minimize the energy expectation value.

We use this methodology to study the confined hydrogen atom, a system described by the confined Coulomb potential. The confining approach is the same as the one used to study the problem of a hydrogenic donor located at the centre of a spherical $GaAs - (Ga, Al)As$ quantum dot, a semiconductor device that confines electrons, [12], [13]. Here the energy of

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the $1s$, $2p$ and $3d$ states of such confined system is evaluated and the results are compared to other variational and exactly numerical results, [13].

II. THE VARIATIONAL METHOD ASSOCIATED TO SQM

Consider a system described by a given potential V_1. The associated Hamiltonian H_1 can be factorized in terms of bosonic operators, in $\hbar = c = 1$ units, [14]- [16].

$$H_1 = -\frac{1}{2}\frac{d^2}{dr^2} + V_1(r) = A_1^+ A_1^- + E_0^{(1)} \tag{1}$$

where $E_0^{(1)}$ is the lowest eigenvalue. Notice that the function $V_1(r)$ includes the barrier potential term. The bosonic operators are defined in terms of the so called superpotential $W_1(r)$,

$$A_1^{\pm} = \frac{1}{\sqrt{2}}\left(\mp\frac{d}{dr} + W_1(r)\right). \tag{2}$$

As a consequence of the factorization of the Hamiltonian H_1, the Riccati equation must be satisfied,

$$W_1^2 - W_1' = 2V_1(r) - 2E_0^{(1)}. \tag{3}$$

Through the superalgebra, the eigenfunction for the lowest state is related to the superpotential W_1 by

$$\Psi_0^{(1)}(r) = Nexp(-\int_0^r W_1(\bar{r})d\bar{r}). \tag{4}$$

At this point we address to the variational method. It was conceived to be an approximative method to evaluate the energy spectra of a given Hamiltonian H and, in particular, its ground state. Its central point is the search for an optimum wave-function $\Psi(r)$ that depends of a number of parameters. This is called the trial wave-function. The approach consists in varying these parameters in the expression for the expectation value of the energy

$$E = \frac{\int \Psi^* H \Psi dr}{\int \mid \Psi \mid^2 dr} \tag{5}$$

until it reaches its minimum value. This value is an upper limit of the energy level pursued.

Thus, using physical arguments an *ansatz* is made to the superpotential and, through the superalgebra, the wave function is evaluated. This is our trial wave function which depends on a set of the free variational parameters, which were introduced by the *ansatz* to the superpotential.

Notice that since the potential is non-exactly solvable, the Hamiltonian is not exactly factorizable, in other words, there is no superpotential that satisfies the Riccati equation exactly. However, the superpotential we have in hands through the *ansatz* does satisfy the Riccati equation by an effective potential, V_{eff}

$$V_{eff}(y) = \frac{\bar{W}_1^2 - \bar{W}_1'}{2} + E(\bar{\mu}) \tag{6}$$

where $\bar{W}_1 = W_1(\bar{\mu})$ is the superpotential that satisfies (3) for $\mu = \bar{\mu}$, the set of parameters that minimise the energy of eq.(5).

III. THE CONFINED COULOMB POTENTIAL

The Hamiltonian of an on-center impurity in a spherical quantum dot can be written in the effective-mass approximation as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\epsilon r} \tag{7}$$

where m^* is the effective mass and ϵ is the dielectric constant of the material of the quantum dot. The donor is assumed to be at the centre of the quantum dot of radius R with an infinite barrier height. This means that the wave function vanishes at $r = R$.

In atomic units, the radial Hamiltonian equation for the Coulomb Potential is given by

$$H = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2}{r}. \tag{8}$$

We use the variational method associated with the SQM in order to get the energy states of the confined atom.

We make the following *ansatz* to the superpotential

$$W(r) = -\frac{c}{r} + b + \frac{a}{R-r} \tag{9}$$

which depends on three free parameters, the variational parameters. From the superalgebra, the eigenfunction obtained from equation (4) is given by

$$\Psi(a,b,c,r) \propto e^{-br}\, r^c\, (R-r)^a. \tag{10}$$

This expression is a trial wavefunction for the variational method having three parameters, a, b and c and vanishing at $r = R$.

The energy is obtained by minimisation of the energy expectation value with respect to the free parameters. The equation to be minimised is given by the following evaluation

$$E(a,b,c) = \frac{\int_0^{R-r} \Psi(a,b,c,r)[-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2}]\Psi(a,b,c,r)dr}{\int_0^{R-r} \Psi(a,b,c,r)dr}. \tag{11}$$

In support of the choice made in (9) for the superpotential are the physical arguments: the first two terms of (9) are related to the exact Coulomb case; the last term is the confining term. This is remarked by the form of the effective potential V_{eff} that satisfies the Riccati equation, (eq. 6), evaluated at the values of a, b, and c that minimize the energy expectation value,

$$V_{eff}(r,a,b,c) = \frac{c(c-1)}{r^2} + \frac{a(a-1)}{(R-r)^2} - \frac{2bc}{r} - \frac{2ac}{r(R-r)} + \frac{2ab}{R-r} + b^2 + \bar{E}(a,b,c)$$

which is infinite at $r = R$.

IV. RESULTS

Thus, minimizing the equation (11) with respect to the parameters a, b and c we find the minimum value of the energy for different values of R and l. These results are shown in the tables bellow. Comparison is made with results from [13], which are based on the standard variational method in which a variational wavefunction is proposed. Ref. [13] also contains exact numerical results.

Table 1. Energy eigenvalues (in Rydbergs) for different values of R for $l = 0$ with a, b and c as variational parameters. Comparison is made with results of Ref. [13].

R	E_{EXACT} Ref. [13]	E_V Ref. [13]	$\frac{\lvert E_{EXACT} - E_V \rvert}{E_{EXACT}}\%$	E_{SQM}	$\frac{\lvert E_{EXACT} - E_{SQM} \rvert}{E_{EXACT}}\%$
0.1	937.986	937.999	0.00	940.688	0.29
0.5	29.496	29.497	0.00	29.571	0.25
1	4.7480	4.7484	0.01	4.7565	0.18
2	-0.25000	-0.24990	0.04	-0.25000	0.00
3	-0.84793	-0.84523	0.32	-0.84706	0.10
4	-0.96653	-0.95518	1.17	-0.96509	0.15

Table 2. Energy eigenvalues (in Rydbergs) for different values of R for $l = 1$ with a, b and c as variational parameters. Comparison is made with results of Ref. [13].

R	E_{EXACT} Ref. [13]	E_V Ref. [13]	$\frac{\lvert E_{EXACT} - E_V \rvert}{E_{EXACT}}\%$	E_{SQM}	$\frac{\lvert E_{EXACT} - E_{SQM} \rvert}{E_{EXACT}}\%$
0.4	116.896	116.925	0.02	117.038	0.12
2.0	3.1520	3.1530	0.03	3.1555	0.11
4.0	0.28705	0.28706	0.00	0.28732	0.09
6.0	-0.111111	-0.11069	0.38	-0.111111	0.00
7.0	-0.17496	-0.17392	0.59	-0.17490	0.03
8.0	-0.20890	-0.20691	0.95	-0.20882	0.04

Table 3. Energy eigenvalues (in Rydbergs) for different values of R for $l = 2$ with a, b and c as variational parameters. Comparison is made with results of Ref. [13].

R	E_{EXACT} Ref. [13]	E_V Ref. [13]	$\frac{\lvert E_{EXACT} - E_V \rvert}{E_{EXACT}}\%$	E_{SQM}	$\frac{\lvert E_{EXACT} - E_{SQM} \rvert}{E_{EXACT}}\%$
1.0	29.935	29.950	0.05	29.958	0.08
3.0	2.5856	2.5867	0.04	2.5876	0.08
4.0	1.2427	1.2431	0.03	1.2437	0.08
5.0	0.65823	0.65836	0.02	0.65873	0.08
7.0	0.19318	0.19318	0.00	0.19333	0.08
8.0	0.09212	0.09216	0.05	0.09220	0.08
12.0	-0.06250	-0.06181	1.11	-0.06250	0.00
14.0	-0.08623	-0.08479	1.66	-0.08622	0.01

V. COMMENTS AND CONCLUSIONS

The variational method associated with SQM was applied to get the energy states of a confined hydrogen atom. The problem is similar to the confinement of electrons in a quantum dot. We used a confining effective potential that depends on tree parameters (a, b, c). Minimizing the energy expectation value with respect to these three parameters we found good results, even for increasing values of the radius R, when compared to results coming from other approximative variational method and exact numerical results. The term $\frac{1}{(R-r)^2}$ in the effective potential leads to border effects, since it is infinite at $R = r$. These effects do not appear in the original problem, eq. (8) and become more perceptive for smaller values of R. For increasing values of R, smaller will be the border effects so that the variational results get better.

In conclusion, we remark that the results presented here once again showed that the association of the superalgebra of SQM with the variational method provides good information about atomic systems.

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